# Pseudospin and spin-spin interactions in ultra-cold alkali atoms

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**Abstract.** Ultra-cold alkali atoms trapped in two distinct hyperfine states in an external magnetic field can mimic magnetic systems of spin 1/2 particles. We describe the spin-dependent effective interaction as a spin-spin interaction. As a consequence of the zero-range, the interaction of spin 1/2 bosons can be described as an Ising or, alternatively, as an XY-coupling. We calculated the spin-spin interaction parameters as a function of the external magnetic field in the Degenerate Internal State (DIS) approximation. We illustrate the advantage of the spin-spin interaction form by mapping the system of N spin 1/2 bosons confined by a tight trapping potential on that of N spin 1/2 spins coupled via an infinite range interaction.

## 1. Introduction

The ability to mimic quantum spins and the promise for controlling their mutual interactions are central ingredients of the cold atom prospects for simulating complex quantum systems: Quantum computation schemes rely on the entanglement of qubits [1], which act as spin $\frac{1}{2}$ objects. Lattice spin models have provided successful descriptions of strongly correlated electron systems [2], usually with the parameters situated near a quantum phase transition so that the systems exhibits quantum critical behavior. A general description of quantum phase transitions has not been devised yet [3] and while scaling arguments have been applied [4], a general renormalization scheme remains an outstanding challenge. The experimental inaccessibility of the condensed strongly correlated electron systems certainly contributes to the challenge of understanding quantum phase transition physics. Cold atom experiments, which offer a very different accessibility and a very different set of control knobs may offer a different and independent laboratory to test concepts. Spin $\frac{1}{2}$ degrees of freedom are also essential building blocks of quantum fluids in regimes that are novel for table-top experiments such as Cooper-paired fermion fluids in the BEC-BCS crossover regime [5, 6, 7], and polarized fermion superfluids (for example, see theory: [8, 9, 10, 11, 12, 13, 14, 15, 16] and experiments: [17, 18, 19, 20, 21, 22].) In addition, bosons trapped in two hyperfine states can act as spin $\frac{1}{2}$ particles [23]. In Bose-Einstein condensates (BEC's) of such particles, the formation of spin $\frac{1}{2}$ magnetic domains has been observed [24], which is a phase separation transition [25].

The observation of spin domain formation [24], of intricate multi-component spin physics in BECs [26], of unstable spin dynamics in spin 1 BECs [27] and the engineering of two-component BEC vortex states [28] and [29] highlight the cold atom ability to access, populate and control hyperfine spin states in cold atom traps. Other experiments demonstrated the cold atom ability to select specific hyperfine spin states in a static, external magnetic field as effective spin components: The above mentioned observation of BEC-phase separation, the probing of the BCS-BEC crossover regime, the spin polarized fermion superfluids, and the recently observed phase transition in an itinerant ferromagnet-like system were all carried out with effective spin $\frac{1}{2}$ particles that occupy a linear combination of hyperfine spin eigenstates in the presence of a static external magnetic field. For reasons we describe below, we refer to the effective spin as 'pseudospin'.

In this paper, we derive the short-range, effective pseudospin-spin interaction potential that describes *s*-wave interactions of ultra-cold atoms that occupy a superposition of two hyperfine states in an external magnetic field. The resulting spin-spin interaction has an anisotropic form, but the commutation or anticommutation relations that respectively characterize bosonic and fermionic systems, combined with the short-range (delta-function) nature of the interaction project the interactions onto the pseudospin triplet subspace for bosons and on the pseudospin singlet subspace for fermions. For bosonic atoms, we find that the inter-particle interactions can be described

by three terms: the first term is a short-range spin independent interaction potential; the second term describes the coupling of one particle's pseudospin to a short-range, spin-independent effective magnetic field carried by the other particle; and the third term is a short-range Ising spin-spin coupling. Alternatively, the spin-spin interaction can be cast into the form of an $XY$-coupling. We show how these terms can be calculated in the Degenerate Internal State (DIS) approximation [30]. We illustrate the advantage of the spin-spin interaction description by deriving the many-spin hamiltonian of N boson particles contained in a tightly confining trap. This system, a controllable quantum magnet, is a promising system to probe macroscopic quantum tunneling, realize spin squeezing and Heisenberg-limited interferometry [31].

## 2. Cold atom spins

The first question to be addressed in simulating one system by another is: what are the salient features of the simulated system that the simulating system needs to possess? As we see below, a spin operator has three components that satisfy a particular commutator algebra. Any operator that satisfies this algebra is a candidate to acts as a spin. We construct the available alkali atom spin states in an external magnetic field explicitly. By selecting two of these states the experimentalists create a cold atom system of effective spin $\frac{1}{2}$ particles.

### *2.1. General spin properties: spin and rotation*

We denote the quantum state of a spin $\overrightarrow{\xi}$ by the spinor $|\xi\rangle$. A spin of amplitude $\xi$, where $\xi$ is an integer or half-integer number, has $2\xi+1$ eigenstates $|\xi_j\rangle$ of the spin projection operator $\hat{\xi}_z\,|\xi_j\rangle = j\,|\xi_j\rangle$ with $j=-\xi,-\xi+1,...,\xi-1,\xi$. The spin operator is the generator of rotations so that under a rotation $\mathcal{R}_{\vec{\epsilon},\alpha}$ by an angle $\alpha$ around the direction of unit vector $\vec{\epsilon}$, the spin state $|\xi\rangle$ (which is a superposition of the states $|\xi_j\rangle$) transforms according to

$$|\mathcal{R}_{\vec{\epsilon},\alpha}\,(\xi)\rangle = \exp\left(i\alpha\vec{\epsilon}\cdot\,\overrightarrow{\xi}\right)|\xi\rangle\,. \tag{1}$$

For an infinitesimal rotation, $\alpha=\delta\alpha\ll 1$, to lowest order in $\delta\alpha$,

$$|\mathcal{R}_{\vec{\epsilon},\delta\alpha}\,(\xi)\rangle \approx \left[1+i\delta\alpha\vec{\epsilon}\cdot\,\overrightarrow{\xi}\right]|\xi\rangle\,. \tag{2}$$

Quantum mechanically, an operator $\mathcal{O}$ in the Hilbert space of a single spin is characterized by its matrix elements $\langle\xi_i|\mathcal{O}|\xi_j\rangle$ where $|\xi_i\rangle$ is the $i$-th element of the $\{\xi_\xi,\xi_{\xi-1},...\}$, basis. We relate the basis matrix elements in the original and in the rotated spinor basis $|\xi_i'\rangle$. When the rotated frame is obtained by rotating around $\vec{\epsilon}$ over an angle $-\delta\alpha$,

$$\langle\xi_i'|\mathcal{O}|\xi_j'\rangle \approx \langle\xi_i|\left(\mathcal{O}-i\;\delta\alpha\;\left[\mathcal{O},\overrightarrow{\epsilon}\cdot\,\overrightarrow{\xi}\right]_-\right)|\xi_j\rangle\;, \tag{3}$$

where the subscript $(-)$ outside the bracket indicates the usual commutator. As a consequence, the operator $\mathcal{O}$ transforms as

$$\mathcal{O}' = \mathcal{O} - i\,\delta\alpha\,\left[\mathcal{O}, \overrightarrow{\epsilon}\cdot\overrightarrow{\xi}\right]_- . \tag{4}$$

Moreover, if the $\mathcal{O}$–operator is rotationally invariant, $\mathcal{O}' = \mathcal{O}$, then $\left[\mathcal{O}, \overrightarrow{\epsilon}\cdot\overrightarrow{\xi}\right]_- = 0$ is the necessary and sufficient condition to ensure that the $\mathcal{O}$–operator is invariant under a rotation around the $\overrightarrow{\epsilon}$-vector.

Classically an infinitesimal rotation transforms a general vector $\overrightarrow{v}$ to $\mathcal{R}_{\overrightarrow{\epsilon},\delta\alpha}(\overrightarrow{v}) = \overrightarrow{v} + \delta\alpha\,\overrightarrow{\epsilon}\times\overrightarrow{v}$. If spin is to act as a vector under a rotation, it is to transform as

$$\mathcal{R}_{\overrightarrow{\epsilon},\delta\alpha}\left(\overrightarrow{\xi}\right) = \overrightarrow{\xi} + \delta\alpha\,\overrightarrow{\epsilon}\times\overrightarrow{\xi}. \tag{5}$$

Choosing $\mathcal{O} = \overrightarrow{\xi}$, by combining Eqs. (4) and (5), and identifying the terms linear in $\delta\alpha$ we obtain

$$i\,\overrightarrow{\epsilon}\,\times\,\overrightarrow{\xi} = \left[\overrightarrow{\xi}, \overrightarrow{\epsilon}\cdot\overrightarrow{\xi}\right]_- . \tag{6}$$

The scalar product of the above vector equality with a unit vector $\overrightarrow{\eta}$ gives

$$\left[\overrightarrow{\xi}\cdot\overrightarrow{\eta}, \overrightarrow{\xi}\cdot\overrightarrow{\epsilon}\right]_- = i\,\overrightarrow{\xi}\cdot(\overrightarrow{\eta}\times\overrightarrow{\epsilon}), \tag{7}$$

and choosing the $\vec{\eta}$ and $\vec{\epsilon}$ vectors as part of a Cartesian $(x, y, z)$ reference frame, $\vec{\eta} = \vec{x}$ and $\vec{\epsilon} = \vec{y}$, we obtain

$$\left[\hat{\xi}_x, \hat{\xi}_y\right]_- = i\,\hat{\xi}_z, \tag{8}$$

the usual form of the angular momentum commutator relation. From this commutator, it can be shown that $\hat{\xi}_x \pm \hat{\xi}_y$ are raising and lowering operators, increasing and decreasing the spin projection eigenvalue of $\hat{\xi}_z$ by one unit. As operators evolve according to the Heisenberg commutator equations in the quantum evolution of the system, any operator satisfying the above commutator relations will evolve as a spin (or angular momentum) of the same Hamiltonian.

The pseudospins we describe below are *not* the generators of rotation and their mutual interactions are *not* rotationally invariant. However, the pseudospins can be described by pseudospin operators that *do* satisfy an angular momentum algebra. In the Heisenberg picture, the quantum equations of motion shows that the dynamics is identical to that of real spins except that the spins and their mutual interactions are *not* rotationally invariant.

### *2.2. The spin structure of alkali atoms in a magnetic field*

Alkali atoms have two spin variables: the electron spin $\mathbf{s}_e$ of magnitude $s_e = \frac{1}{2}$ carried by the $s$-wave valence electron and the nuclear spin $\mathbf{i}$ of magnitude $i$. The electron 'spins' in the magnetic field of the nucleus and the short-range part of the nuclear spin's magnetic field (the Fermi contact term) contributes to the energy in a first-order perturbation

calculation [32]. The corresponding contribution takes the form $a_{hf}\mathbf{i}\cdot\mathbf{s}_e$, which is the hyperfine interaction. We refer to $a_{hf}$ as the hyperfine energy.

In a static, external, homogeneous magnetic field $\mathbf{B}$ of strength $B$, $\mathbf{B} = B\mathbf{z}$, the interaction of the electronic and nuclear spins with the magnetic field and with each other are described by the Zeeman spin Hamiltonian

$$\mathcal{H} = B\mathbf{z}\cdot[\mu_e\mathbf{s}_e - \mu_N\mathbf{i}] + a_{hf}\mathbf{s}_e\cdot\mathbf{i}, \tag{9}$$

where $\mu_e = \hbar/2m_ec$, $\mu_N = \hbar/2m_pc$ represent the electronic and nuclear Bohr magneton, respectively, with $m_e$ for the electron mass and $m_p$ for the proton mass. As the nucleons are heavier and the nuclear Bohr magneton, $\mu_N$, proportionally smaller (by three orders of magnitude) than $\mu_e$, $\mu_N$ and we neglect it for now. Scaling the magnetic field strength in units of the hyperfine field $B_{hf} = a_{hf}/\mu_e$, $b = B/B_{hf}$, the Zeeman Hamiltonian takes the form

$$\frac{\mathcal{H}}{a_{hf}} = \mathbf{s}_e\cdot\mathbf{i} + b\ \mathbf{z}\cdot\mathbf{s}_e. \tag{10}$$

At zero magnetic field, $b = 0$, the structure of the spin Hamiltonian eigenstates is most readily analyzed by introducing the total hyperfine spin operator, $\mathbf{f} = \mathbf{i} + \mathbf{s}_e$. The Hamiltonian eigenstates can be chosen to be eigenstates of good ($\mathbf{f}^2$) and $\mathbf{f}\cdot\mathbf{z}$ quantum numbers. The eigenvalues of the $\mathbf{f}^2$ operator are $f\,(f+1)$, with $f = i \pm 1/2$. The eigenvalues of the $\mathbf{f}\cdot\mathbf{z}$ are labeled by the eigenvalue $m_f$. The $|f, m_f\rangle$ states of the same $f$-quantum number are degenerate. The first term of Eq. (10) can be written as $\left(\mathbf{f}^2 - \mathbf{s}_e^2 - \mathbf{i}^2\right)/2$, and when $b = 0$, $E(f, m_f, b) = E_0(f)$ and $E_0(f = i+1/2) = a_{hf}i/2$ and $E_0(f = i - 1/2) = -a_{hf}(i+1)/2$, giving a hyperfine splitting $a_{hf}(i + \frac{1}{2})$. This splitting is determined spectroscopically. For example, $^{23}Na$ has a hyperfine energy measured to be $a_{hf} = 42.5mK = 0.95GHz$ (which greatly exceeds cold atom trap depths $\sim \mu K$), corresponding to a hyperfine magnetic field strength equal to $B_{hf} \approx 709G$.

At finite magnetic field, $f$ is not a good quantum number, but it is convenient and customary to refer to the $f$-value that the same state takes on in the adiabatic $b \to 0$-limit. On the other hand, the total spin projection, $m_f$ remains a good quantum number. We parametrize the corresponding state by an angle $\theta$ as

$$\begin{aligned}\left|f^{\pm}, m_f\right\rangle \;=\; &\pm\cos\left(\frac{\theta^{\pm}}{2}\right)\left|m_i = m_f - \frac{1}{2}, m_e = +\frac{1}{2}\right\rangle \\ &+\sin\left(\frac{\theta^{\pm}}{2}\right)\left|m_i = m_f + \frac{1}{2}, m_e = -\frac{1}{2}\right\rangle.\end{aligned} \tag{11}$$

We restrict the range of $\theta$-angles to the $[0, \pi]$ interval, allowing for coefficients of a different sign by adding $\pm$ explicitly to the cosine term. By parametrizing the state as in Eq. (11), the $\theta$ is also the inclination angle of the average electron spin vector in that hyperfine state. The optimal value of $\theta$ depends on the spin projection eigenvalue $m_f$.

Using the angular momentum algebra Eq. (8), the spin product expectation value $\langle\mathbf{s}_e\cdot\mathbf{i}\rangle$, of the states of Eq. (11) give

$$\langle\mathbf{s}_e\cdot\mathbf{i}\rangle = \frac{1}{2}\left[\cos(\theta)\, m_f \pm \sin(\theta)\sqrt{\left(i+\frac{1}{2}\right)^2 - m_f^2}\right] - \frac{1}{4}, \tag{12}$$

where, $\pm$ refer to the relative sign of the electron spin up and down components, as introduced in (11). Taking the extreme of the expectation value of Eq. (10) with respect to $\theta$ in (11) gives

$$\frac{E(\pm, m_f)}{a_{hf}} = (b + m_f)\cos(\theta) \pm \sin(\theta)\sqrt{\left(i + \frac{1}{2}\right)^2 - m_f^2} - \frac{1}{4}, \tag{13}$$

and by requiring $\partial E/\partial\theta = 0$, we obtain the optimal inclination angle $\tan(\theta^{\pm})$,

$$\tan\left(\theta^{\pm}\right) = \pm\frac{\sqrt{\left(i + \frac{1}{2}\right)^2 - m_f^2}}{(b + m_f)}. \tag{14}$$

As $b \gg 1$, $\tan(\theta^{\pm}) \to \pm[i+1]/b \to \pm\infty$, corresponding to $\theta^+ \to 0$ and $\theta^- \to \pi$: the electron spin in hyperfine states align or anti-align with the external magnetic field when the strength of that field significantly exceeds the hyperfine field strength. For notational convenience we introduce the square root of the sum of the squares of the numerator and denominator,

$$e(m_f, b) = \sqrt{b^2 + 2m_f b + \left(i + \frac{1}{2}\right)^2}. \tag{15}$$

Then the angular projections can be written as

$$\cos\left(\theta^{\pm}\right) = \pm\frac{(b + m_f)}{e(m_f, b)}, \qquad \sin\left(\theta^{\pm}\right) = \frac{\sqrt{(i + 1/2)^2 - (m_f)^2}}{e(m_f, b)}. \tag{16}$$

Substitution of Eq. (16) into Eq. (10) yields the Zeeman eigenenergies $E(\pm, m_f, b)$ ,

$$\frac{E(\pm, m_f, b)}{a_{hf}} = \pm\frac{e(m_f, b)}{2} - 1/4, \tag{17}$$

where the superscripts $\pm$ are now seen to indicate whether the hyperfine state belongs to the $f^+ = i + 1/2$ or the $f^- = i - 1/2$–superpositions of Eq. (11). To see that, note that in the limit of vanishing magnetic field, $\lim_{b\to 0}$, $e(m_f, b) \to i + 1/2$, so that $E(+, m_f, b)$ approaches $E_0(f = i + 1/2) = a_{hf} i/2$ while $E(-, m_f, b)$ approaches $E_0(f = i - 1/2) = -a_{hf}[i+1]/2$. Actually, the expression Eq. (17 ) describes the 'non-stretched' states, $|m_f| < i + 1/2$. For the stretched states $|f = i + 1/2, m_f = i + 1/2\rangle$ and $|f = i + 1/2, m_f = -i - 1/2\rangle$,

$$\frac{E(f^+, m_f = \pm f^+, b)}{a_{hf}} = \pm\frac{b}{2} + \frac{i}{2}, \tag{18}$$

corresponding to $\theta = 0$ and $\theta = \pi$ in the linear superpositions of Eq. (11). In Fig. 1, we show the magnetic field dependence of the spin states for the nuclear spin value $i = \frac{3}{2}$ that describes $^7Li$, $^{23}Na$ and $^{87}Rb$, three of the most used cold atom alkali atom species.

The electron spin expectation value $\langle \mathbf{s}_e \rangle$,

$$\langle f, m_f | \mathbf{s}_e | f, m_f \rangle = \mathbf{z}\frac{\cos(\theta)}{2} = \pm\mathbf{z}\frac{(b + m_f)}{2e(m_f, b)}, \tag{19}$$

points in the direction of the external magnetic field.

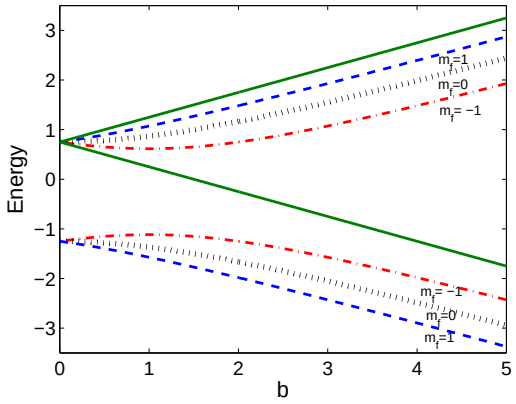


**Figure 1.** Hyperfine energy levels for nuclear spin $i = 3/2$, the nuclear spin magnitude of bosonic atoms such as $^7Li$, $^{23}Na$ and $^{87}Rb$.

### *2.3. Pseudospin*

By trapping cold atoms in a specific hyperfine state in an external magnetic field and by coherently transferring part of the spin population into a different hyperfine state, either by accessing a laser-driven two-photon Raman transition or by means of another magnetic field that is oscillating near the energy-difference, the experimentalists prepare the atoms in a superposition of two hyperfine states, $|f_1, m_{f_1}\rangle$ and $|f_2, m_{f_2}\rangle$. If the hyperfine states have been selected to ensure that no other spin states couple, $|f_1, m_{f_1}\rangle$ and $|f_2, m_{f_2}\rangle$ act as the basis of an effective spin $\frac{1}{2}$. We can than assign one the role of 'spin-up' the other that of 'spin-down' state, $|f_1, m_{f_1}\rangle = |\uparrow\rangle$ and $|f_2, m_{f_2}\rangle = |\downarrow\rangle$. Interestingly, if the atoms are bosonic, i.e. if their hyperfine spin $f$ takes on an integer value, the atoms become effective spin $\frac{1}{2}$ bosons.

The coupling to other hyperfine states has to be avoided because not only does the role of additional hyperfine states require a larger Hilbert space description, but also it generally causes significant particle loss. For magnetic field strengths near the hyperfine magnetic field, $b \sim 1$, the Zeeman levels are widely spaced with energy differences comparable to $a_{hf}$ (tens of $mK$), considerably larger than the typical trap depths ($\mu K$). Hence, spin flip collisions in which particles end up in lower energy spin states create particle pairs of sufficient kinetic energy to evict spin flipped particles from the trap. However, conservation of energy and conservation of total spin projection ($m_f$) in binary atom interactions limit the spin-changing collisions that can take place in an external magnetic field.

In the case of nuclear spin $i = \frac{3}{2}$, the experimentalist can select either the two lowest or the two highest energy levels of the $f = 1$ manifold: either $|1, 0\rangle$ and $|1, -1\rangle$ or $|1, 0\rangle$ and $|1, +1\rangle$. While collisions $|1, 0\rangle + |1, 0\rangle \rightarrow |1, -1\rangle + |1, +1\rangle$ would produce spin states not included in the spin-up and spin-down basis, in the region $b \sim 1$, the energy cost of a spin flip up ($m_f$ from 0 to $+1$) outweighs the energy gain from the corresponding spin flip down process ($m_f$ from 0 to $-1$), as can be seen from Fig. 1 so

that this process is energy forbidden. For nuclear spin 1, $i = 1$, as in the case of $^6Li$, $^{23}$Na and $^{87}$Rb, the experimentalist can select the two lowest energy hyperfine states, $|\uparrow\rangle = |\frac{1}{2}, \frac{1}{2}\rangle$, and $|\downarrow\rangle = \left|\frac{1}{2}, -\frac{1}{2}\right\rangle$, for instance.

In the $|f_1, m_{f_1}\rangle = |\uparrow\rangle$ and $|f_2, m_{f_2}\rangle = |\downarrow\rangle$ basis the pseudospin operator takes the form $\mathbf{s} = \frac{1}{2}\sigma$, where $\sigma$ is the Pauli-spin vector operator, $\sigma = \sigma_x\mathbf{x} + \sigma_y\mathbf{y} + \sigma_z\mathbf{z}$, with $\sigma_x$, $\sigma_y$, and $\sigma_z$ the Pauli spin matrices. Note that $\mathbf{s}$ is *not* the generator of rotations. Under rotation, the spin components do not transform among each other according to Eq. (1), although the $\mathbf{s}$ components still satisfy angular momentum commutator relations $[s_x, s_y]_- = is_z$. Therefore, the time evolution of the many-spin system (governed by commutation relations in the Heisenberg picture) is indistinguishable from the quantum evolution of the magnetic many-spin system of the same parameters. The concept of effective spin parallels closely that of iso-spin in nuclear physics [33], except that a Raman transition and/or oscillating magnetic field can convert spin-down into spin-up particles. Likewise, as emphasized by Bloch [34], any two-state system (and its decoherence) can be described by an effective spin $\frac{1}{2}$ system.

To picture the role of the pseudo-spin direction, we parametrize an arbitrary, normalized two component spinor $|\xi_{ps}\rangle$ by introducing two angles $\theta$ and $\phi$.

$$|\xi_{ps}\rangle = \begin{pmatrix} \xi_\uparrow \\ \xi_\downarrow \end{pmatrix} = \begin{pmatrix} e^{i\frac{\phi}{2}} \cos\frac{\theta}{2} \\ e^{-i\frac{\phi}{2}} \sin\frac{\theta}{2} \end{pmatrix}. \tag{20}$$

In this notation, $\phi$ denotes the relative phase: the difference of the complex phase of the 'up' amplitude and of that of the 'down' amplitude. Also, $\cos\theta$ denotes the effective polarization: the difference between the up probability and the down probability. Then the expectation value of the effective spin vector $\langle\mathbf{s}\rangle$ in terms of $\theta$ and $\phi$ is

$$\langle\mathbf{s}\rangle = \frac{1}{2}\langle\xi_{ps}|\,\vec{\sigma}\,|\xi_{ps}\rangle = \frac{1}{2}\left(\sin\theta\cos\phi\mathbf{x} + \sin\theta\sin\phi\mathbf{y} + \cos\theta\mathbf{z}\right), \tag{21}$$

which is a vector on the surface of a sphere of radius $\frac{1}{2}$ (known as the 'Bloch sphere'). The inclination $\theta$ and azimuthal $\phi$ angles of the expectation value of the pseudospin vector then respectively characterize the 'polarization' and the phase difference. If an ensemble measurement reveals $N_{\uparrow(\downarrow)}$ atoms in the 'up' ('down') hyperfine state, then $\langle\cos(\theta)\rangle = (N_\uparrow - N_\downarrow)\,/\,(N_\uparrow + N_\downarrow)$.

## 3. Spin-spin binary atom interactions

Cold alkali atoms are interesting building blocks for simulating magnetic systems: their mutual interactions preserve the overall spin projection (the sum of $m_f$ is preserved), the interactions are naturally spin dependent and the strength of these interactions and their spin-dependence can be varied by a Feshbach resonance. We write the effective atom-atom interaction as a spin-spin interaction. The statistics of indistinguishability, combined with the short-range nature of the effective interaction gives a short-range Ising-like spin-spin interaction or, alternatively, a short-range $XY$-interaction. We calculate the spin-dependence in the Degenerate Internal State (DIS) approximation.

### *3.1. Effective inter-particle interaction in pseudospin language*

In cold atom experiments, the length scales relevant to the many-body physics description ($\sim \mu m$) significantly exceed the length scale on which the atoms interact (which ranges from Bohr-radius to $nm$). As a consequence, the interactions of indistinguishable atoms $i$ and $j$ with position coordinates $\mathbf{x}_i$ and $\mathbf{x}_j$ can be described by an effective contact interaction potential

$$V\left(\mathbf{x}_i, \mathbf{x}_j\right) = \frac{4\pi\hbar^2}{m} a \delta\left(\mathbf{x}_i - \mathbf{x}_j\right). \tag{22}$$

where $a$ denotes the scattering length and $m$ represents the single particle mass. In the low energy regime of interest in a many-body description, this interaction reproduces the real binary atom scattering physics (to all orders) in a first order perturbation calculation. The interaction potential reproduces the correct binary atom s-wave scattering amplitude in the Born approximation. Introducing the annihilation (creation) field operators $\hat{\psi}$ ($\hat{\psi}^\dagger$), the particle-particle interactions are described by

$$\begin{aligned}\hat{H}_{int} &= \frac{1}{2}\int d^3x \int d^3x' \;\; \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}')V\left(\mathbf{x}-\mathbf{x}'\right)\hat{\psi}(\mathbf{x}')\hat{\psi}(\mathbf{x}) \\ &= \frac{1}{2}\left(\frac{4\pi\hbar^2}{m}\right)\int d^3x \;\; \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\psi}(\mathbf{x}) \,,\end{aligned} \tag{23}$$

in the Hamiltonian operator. When the indistinguishable particles are bosons that occupy two possible spin states, $|\uparrow\rangle$ and $|\downarrow\rangle$, we distinguish interactions between particles in like spin states, described by a scattering length $a_\uparrow$ ($a_\downarrow$) if that state is the 'up' ('down') spin-state, and between particles in unlike spin states, described by scattering length $a_u$. The Hamiltonian operator that accounts for these interactions takes the form

$$\begin{aligned}\hat{H}_{int} = \frac{1}{2}\left(\frac{4\pi\hbar^2}{m}\right)\Bigg(& a_\uparrow \int d^3x \;\; \hat{\psi}^\dagger_\uparrow(\mathbf{x})\hat{\psi}^\dagger_\uparrow(\mathbf{x})\hat{\psi}_\uparrow(\mathbf{x})\hat{\psi}_\uparrow(\mathbf{x}) \\ &+ a_\downarrow \int d^3x \;\; \hat{\psi}^\dagger_\downarrow(\mathbf{x})\hat{\psi}^\dagger_\downarrow(\mathbf{x})\hat{\psi}_\downarrow(\mathbf{x})\hat{\psi}_\downarrow(\mathbf{x}) \\ &+ 2a_u \int d^3x \;\; \hat{\psi}^\dagger_\uparrow(\mathbf{x})\hat{\psi}^\dagger_\downarrow(\mathbf{x})\hat{\psi}_\downarrow(\mathbf{x})\hat{\psi}_\uparrow(\mathbf{x})\Bigg).\end{aligned} \tag{24}$$

By virtue of Pauli exclusion principle, fermion particles occupying two spin states $|\uparrow\rangle$ and $|\downarrow\rangle$ only interact via short-ranged interactions if they are in different spin states,

$$\hat{H}_{int} = \left(\frac{4\pi\hbar^2 a_F}{m}\right)\int d^3x \;\; \hat{\psi}^\dagger_\uparrow(\mathbf{x})\hat{\psi}^\dagger_\downarrow(\mathbf{x})\hat{\psi}_\downarrow(\mathbf{x})\hat{\psi}_\uparrow(\mathbf{x}) \,, \tag{25}$$

where $a_F$ describes the low energy fermion-fermion scattering. We obtain these expressions from a scattering picture and derive a pseudo spin-spin form of the particle-particle effective interaction potentials.

If the effective pseudo spin projection is conserved, interacting spin $\frac{1}{2}$ atoms, 1 and 2, can undergo four types of scattering events, represented in Fig. 2, $|\uparrow\uparrow\rangle \to |\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle \to |\downarrow\downarrow\rangle$, $|\uparrow\downarrow\rangle \to |\uparrow\downarrow\rangle$ (with the same amplitude as $|\downarrow\uparrow\rangle \to |\downarrow\uparrow\rangle$ ) and $|\downarrow\uparrow\rangle \to |\uparrow\downarrow\rangle$, (with the same amplitude as $|\uparrow\downarrow\rangle \to |\downarrow\uparrow\rangle$ ) where the first arrow in the brackets indicates

the spin of atom 1, the second arrow shows the spin of atom 2. By construction, the effective interaction yields the correct transition matrix elements in the Born-approximation for the four types of binary atom scattering events: $(4\pi\hbar^2 a_\downarrow/m)$ for the mutual scattering of two 'down' particles, $(4\pi\hbar^2 a_\uparrow/m)$ for the mutual scattering of two 'up' particles, $(4\pi\hbar^2 a_D/m)$ for direct scattering (unlike spin scattering without spin flip) and $(4\pi\hbar^2 a_x/m)$ for exchange scattering events (unlike spin scattering with spin flip).

Denoting the full coordinate of particle $i$, which consists of position $\mathbf{x}_i$ and spin $\mathbf{s}_i$ by $\mathbf{r}_i$, we can replace the effective interaction potential Eq. (22) by

$$V(\mathbf{r}_1, \mathbf{r}_2) = \frac{4\pi\hbar^2}{m}\hat{a}\delta(\mathbf{x}_1 - \mathbf{x}_2), \tag{26}$$

which is a spin-operator. In the basis of the up and down spins, $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$, the $\hat{a}$-operator reads

$$\hat{a} = \begin{pmatrix} a_\uparrow & 0 & 0 & 0 \\ 0 & a_D & a_x & 0 \\ 0 & a_x & a_D & 0 \\ 0 & 0 & 0 & a_\downarrow \end{pmatrix}, \tag{27}$$

in accordance with the above description.

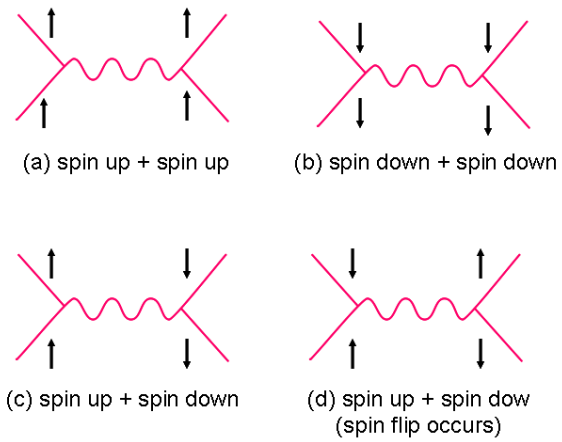


**Figure 2.** Graphic illustration of the four types of binary atom scattering processes: (a) two spin-up particles collide, (b) two spin down particles collide, (c) one spin up and one spin-down particle particle scatter while the spin projection of the interacting particles remains the same, and (d) a spin-up and a spin-down particle exchange spin states in the collision.

To connect with spin physics we write the spin dependent scattering length operator, $\hat{a}$, as the sum of products of single particle spin-operators. We write Eq. (27) as

$$\hat{a} = a_o\hat{I} + a_{z,+}(s_{1,z} + s_{2,z}) + a_{z,p}[4(s_{1,z}s_{2,z})] + a_x[2(s_{1,x}s_{2,x} + s_{1,y}s_{2,y})], \tag{28}$$

where $\hat{I}$ denotes the unit operator. The operators in square brackets are the spin projection sum operator,

$$s_{1,z} + s_{2,z} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \tag{29}$$

the spin projection product operator,

$$s_{1,z}s_{2,z} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{30}$$

and the exchange operator,

$$s_{1,x}s_{2,x} + s_{1,y}s_{2,y} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{31}$$

By comparing the off-diagonal matrix elements, it is clear that the exchange operator coefficient must be equal to the exchange scattering length $a_x$. Identifying the diagonal matrix elements we find $a_o, a_{z,p}, a_{z,+}$;

$$\begin{aligned} a_o &= \frac{a_\uparrow + a_\downarrow + 2a_D}{4}, \\ a_{z,p} &= \frac{a_\uparrow + a_\downarrow - 2a_D}{4}, \\ a_{z,+} &= \frac{a_\uparrow - a_\downarrow}{2}\ . \end{aligned} \tag{32}$$

Hence, the expression

$$\begin{aligned} V(\vec{r}_1, \vec{r}_2) = \left(\frac{4\pi\hbar^2}{m}\right) \delta(\mathbf{x}_1 - \mathbf{x}_2) \Bigg\{ \left[\frac{a_\uparrow + a_\downarrow + 2a_D}{4}\right] + \left[\frac{a_\uparrow - a_\downarrow}{2}\right] (s_{1,z} + s_{2,z}) \\ + \left[a_\uparrow + a_\downarrow - 2a_D\right] (s_{1,z}s_{2,z}) + 2a_x \left(s_{1,x}s_{2,x} + s_{1,y}s_{2,y}\right) \Bigg\}. \end{aligned} \tag{33}$$

translates the effective interaction potential operator Eq. (26) into pseudo-spin language.

### *3.2. A magnetic-like interaction form of the inter-particle interactions*

In the interest of exploiting the magnetism analogy, we note that the effective spin-dependent interaction Eq. (33) can be rephrased as a magnetic interaction. Specifically, the spin-dependent part stems from the interaction of the effective spin of one particle with an effective short-ranged magnetic field carried by the other particle. That description allows one to interpret the interaction of one particle in a many-body system to be caused by the interaction with an external field and with an internal magnetic field generated by the moments of the other particles.

We write the effective interaction of atoms 1 and 2, as the sum of a spin independent contact interaction, $V_o$ and and a spin interaction, $V_s$, $V(\vec{r}_1, \vec{r}_2) = V_o(\vec{x}_1 - \vec{x}_2) + V_s(\vec{r}_1, \vec{r}_2)$ where

$$V_o(\mathbf{x}_1 - \mathbf{x}_2) = \frac{\pi\hbar^2}{m}(a_\uparrow + a_\downarrow + 2a_D)\,\delta(\mathbf{x}_1 - \mathbf{x}_2). \tag{34}$$

The spin-dependent part we cast into the form of the energy of a spin in a magnetic field with unit effective Bohr-magneton (as we chose the spin to be dimensionless, the effective magnetic field than takes the units of energy)

$$V_s(\mathbf{r}_1, \mathbf{r}_2) = \mathbf{s}_1 \cdot \mathbf{h}_2(\mathbf{x}_1) + \mathbf{s}_2 \cdot \mathbf{h}_1(\mathbf{x}_2), \tag{35}$$

where we assume the effective **h**–magnetic field to be the short-range part of an effective moment **m**,

$$\mathbf{h}_i(\mathbf{x}) = \mathbf{m}_i \delta(\mathbf{x} - \mathbf{x}_i). \tag{36}$$

The effective **m**-moment is an operator,

$$\mathbf{m}_i = m_{s,o}\mathbf{z} + m_{s,\parallel}\mathbf{z}\ (\ \mathbf{s}_i\ \cdot \mathbf{z}\ ) + m_{s,\perp}\ \mathbf{z} \times (\ \mathbf{s}_i \times \mathbf{z}\ ), \tag{37}$$

with moment parameters

$$\begin{aligned} m_{s,o} &= \frac{2\pi\hbar^2}{m}(a_\uparrow - a_\downarrow), \\ m_{s,\parallel} &= \frac{2\pi\hbar^2}{m}(a_\uparrow + a_\downarrow - 2a_D), \\ m_{s,\perp} &= \frac{4\pi\hbar^2}{m}a_x, \end{aligned} \tag{38}$$

that depend on the scattering lengths.

### *3.3. The effect of quantum statistics on short-range spin-spin interactions*

As the pseudo spin operators are not the generators of rotations, the spin-spin interaction can be and generally is anisotropic. The $m_o$-term describes the interaction of $\vec{s}$ with an effective short-range magnetic moment that points in the $\vec{z}$-direction (the direction of the physical magnetic field, the actual field that splits the Zeeman-levels) and is independent of the pseudo-spin of the particle that carries the moment. Another source of anisotropy is the difference in the $m_\parallel$ and $m_\perp$-moment parameters. The short-range nature of the interactions and the quantum statistics of the interacting particles, give a moment that can be chosen to align itself with the magnetic field direction or to be perpendicular to it. To see that, consider the interaction

$$\hat{H}_{int} = \frac{1}{2}\left(\frac{4\pi\hbar^2}{m}\right)\int d^3x\ \left\langle \hat{\psi}^\dagger(\vec{x})\,\hat{\psi}^\dagger(\vec{x})\,|\hat{a}|\,\hat{\psi}(\vec{x})\,\hat{\psi}(\vec{x})\right\rangle, \tag{39}$$

where $\hat{a}$ denotes the spin-dependent scattering length operator of Eq. (27), where

$$|\hat{\psi}(\vec{x})\,\hat{\psi}(\vec{x})\rangle = \begin{pmatrix} \hat{\psi}_\uparrow(\vec{x})\,\hat{\psi}_\uparrow(\vec{x}) \\ \hat{\psi}_\uparrow(\vec{x})\,\hat{\psi}_\downarrow(\vec{x}) \\ \hat{\psi}_\downarrow(\vec{x})\,\hat{\psi}_\uparrow(\vec{x}) \\ \hat{\psi}_\downarrow(\vec{x})\,\hat{\psi}_\downarrow(\vec{x}) \end{pmatrix}, \tag{40}$$

indicates the two-particle spinor. The short-range nature of the interaction causes the field operators to be evaluated at the same position, $\vec{x}$. As pairs of annihilation and creation operators of the same argument, the two-particle spinor components obey commutator (anti-commutator) relations if the interacting particles are bosonic (fermionic), $\hat{\psi}_i(\vec{x})\,\hat{\psi}_j(\vec{x}) = \pm\hat{\psi}_j(\vec{x})\,\hat{\psi}_i(\vec{x})$. By writing the components of the two particle spinor Eq. (40) as half the sum with itself, then replacing the second term by $\pm$ its reverse order, we obtain, for bosons

$$\left|\hat{\psi}(\vec{x})\,\hat{\psi}(\vec{x})\right\rangle = \begin{pmatrix} \hat{\psi}_\uparrow(\vec{x})\,\hat{\psi}_\uparrow(\vec{x}) \\ \frac{1}{\sqrt{2}}\left(\frac{\hat{\psi}_\uparrow(\vec{x})\hat{\psi}_\downarrow(\vec{x})+\hat{\psi}_\downarrow(\vec{x})\hat{\psi}_\uparrow(\vec{x})}{\sqrt{2}}\right) \\ \frac{1}{\sqrt{2}}\left(\frac{\hat{\psi}_\downarrow(\vec{x})\hat{\psi}_\uparrow(\vec{x})+\hat{\psi}_\uparrow(\vec{x})\hat{\psi}_\downarrow(\vec{x})}{\sqrt{2}}\right) \\ \hat{\psi}_\downarrow(\vec{x})\,\hat{\psi}_\downarrow(\vec{x}) \end{pmatrix}, \tag{41}$$

for bosons and for fermions

$$\left|\hat{\psi}(\vec{x})\,\hat{\psi}(\vec{x})\right\rangle = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}}\left(\frac{\hat{\psi}_\uparrow(\vec{x})\hat{\psi}_\downarrow(\vec{x})-\hat{\psi}_\downarrow(\vec{x})\hat{\psi}_\uparrow(\vec{x})}{\sqrt{2}}\right) \\ \frac{1}{\sqrt{2}}\left(\frac{\hat{\psi}_\downarrow(\vec{x})\hat{\psi}_\uparrow(\vec{x})-\hat{\psi}_\uparrow(\vec{x})\hat{\psi}_\downarrow(\vec{x})}{\sqrt{2}}\right) \\ 0 \end{pmatrix}. \tag{42}$$

The resulting non-vanishing column matrix elements are components of the pseudo-spin triplet manifold in the boson-case and the pseudospin singlet state in the fermion case. We find that the two-particle spinor is projected onto the triplet subspace if the fields are bosonic and onto the singlet subspace if the fields are fermionic,

$$\begin{aligned} \left|\hat{\psi}(\vec{x})\,\hat{\psi}(\vec{x})\right\rangle_{bosons} &= \hat{\Pi}_T\left|\hat{\psi}(\vec{x})\,\hat{\psi}(\vec{x})\right\rangle, \\ \left|\hat{\psi}(\vec{x})\,\hat{\psi}(\vec{x})\right\rangle_{fermions} &= \hat{\Pi}_S\left|\hat{\psi}(\vec{x})\,\hat{\psi}(\vec{x})\right\rangle, \end{aligned} \tag{43}$$

where the $\hat{\Pi}_T$ ($\hat{\Pi}_S$) project onto the two-particle pseudospin triplet (singlet) subspace. We can check that statement by direct inspection. For instance, the second component of the column matrices Eq. (41) and Eq. (42) represents the two-particle annihilation field of the $|\uparrow\downarrow\rangle$–state, which can be written as $|\uparrow\downarrow\rangle = \frac{1}{\sqrt{2}}\left(\frac{|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle}{\sqrt{2}} + \frac{|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle}{\sqrt{2}}\right)$, so that $\hat{\Pi}_T|\uparrow\downarrow\rangle = \frac{1}{\sqrt{2}}\frac{|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle}{\sqrt{2}}$ and $\hat{\Pi}_S|\uparrow\downarrow\rangle = \frac{1}{\sqrt{2}}\frac{|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle}{\sqrt{2}}$, corresponding to the spin states of the second component of the right-hand sides of Eqs. (41) and (42).

Writing the boson matrix product of the interaction Hamiltonian out, we find that we can also write the effective interaction Hamiltonian as a bracket of the triplet two-particle spinor,

$$\left|\hat{\psi}(\vec{x})\,\hat{\psi}(\vec{x})\right\rangle_T = \begin{pmatrix} \hat{\psi}_\uparrow(\vec{x})\,\hat{\psi}_\uparrow(\vec{x}) \\ \frac{\hat{\psi}_\uparrow(\vec{x})\hat{\psi}_\downarrow(\vec{x})+\hat{\psi}_\downarrow(\vec{x})\hat{\psi}_\uparrow(\vec{x})}{\sqrt{2}} \\ \hat{\psi}_\downarrow(\vec{x})\,\hat{\psi}_\downarrow(\vec{x}) \end{pmatrix}, \tag{44}$$

in terms of which

$$\hat{H}_{int} = \frac{1}{2}\left(\frac{4\pi\hbar^2}{m}\right)\int d^3x \;\; {}_T\left\langle\hat{\psi}^\dagger(\vec{x})\,\hat{\psi}^\dagger(\vec{x})\,|\hat{a}_T|\hat{\psi}(\vec{x})\,\hat{\psi}(\vec{x})\right\rangle_T, \tag{45}$$

where the triplet scattering length operator $\hat{a}_T$ is now represented by a diagonal matrix,

$$\hat{a} = \begin{pmatrix} a_\uparrow & 0 & 0 \\ 0 & a_D + a_x & 0 \\ 0 & 0 & a_\downarrow \end{pmatrix}. \tag{46}$$

One more application of the commutator relations casts the interaction Hamiltonian Eq. (45) in the form of Eq. (24) provided we identify the unlike boson scattering length $a_u$ with $a_u = a_D + a_x$. Likewise, the fermion interaction

$$\hat{H}_{int} = \frac{1}{2}\left(\frac{4\pi\hbar^2}{m}\right)\int d^3x \;\; {}_S\left\langle \hat{\psi}^\dagger(\vec{x})\,\hat{\psi}^\dagger(\vec{x})\,|\hat{a}_S|\hat{\psi}(\vec{x})\,\hat{\psi}(\vec{x})\right\rangle_S, \tag{47}$$

with two-particle singlet spin component

$$\left|\hat{\psi}(\vec{x})\,\hat{\psi}(\vec{x})\right\rangle_S = \frac{\hat{\psi}_\uparrow(\vec{x})\,\hat{\psi}_\downarrow(\vec{x}) - \hat{\psi}_\downarrow(\vec{x})\,\hat{\psi}_\uparrow(\vec{x})}{\sqrt{2}}\,, \tag{48}$$

and singlet scattering length,

$$\hat{a}_S = a_D - a_x\,, \tag{49}$$

reduces to the form of Eq. (25) if we identify $a_F$ with $a_F = a_D - a_x$.

As an interesting consequence of the triplet projection caused by boson statistics, the spin-spin interaction can be written in two equivalent forms. As $\vec{s}_1 \cdot \vec{s}_2 = 1/4$ in a triplet state, we can either replace $s_{1,z}s_{2,z} = 1/4 - (s_{1,x}s_{2,x} + s_{1,y}s_{2,y})$ or, alternatively, $s_{1,x}s_{2,x} + s_{1,y}s_{2,y}$ by $s_{1,x}s_{2,x} + s_{1,y}s_{2,y} = 1/4 - s_{1,z}s_{2,z}$. As a consequence of the second replacement, the effective spin-spin interaction takes the form of a short-range Ising-like interaction, the second replacement gives a short-range XY spin-spin interaction. The resulting boson spin-spin interactions

$$\begin{aligned} V_I(\vec{r}_1,\vec{r}_2) \;=\; & \left(\frac{4\pi\hbar^2}{m}\right)\delta(\vec{x}_1-\vec{x}_2)\left\{\left[\frac{a_\uparrow + a_\downarrow + 2a_u}{4}\right]\right. \\ & \left. + \left[\frac{a_\uparrow - a_\downarrow}{2}\right](s_{1,z}+s_{2,z}) + [a_\uparrow + a_\downarrow - 2a_u](s_{1,z}s_{2,z})\right\}, \end{aligned} \tag{50}$$

and

$$\begin{aligned} V_{XY}(\vec{r}_1,\vec{r}_2) \;=\; & \left(\frac{4\pi\hbar^2}{m}\right)\delta(\vec{x}_1-\vec{x}_2)\left\{\left[\frac{a_\uparrow + a_\downarrow}{2}\right] + \left[\frac{a_\uparrow - a_\downarrow}{2}\right](s_{1,z}+s_{2,z})\right. \\ & \left. - [a_\uparrow + a_\downarrow - 2a_u](s_{1,x}s_{2,x} + s_{1,y}s_{2,y})\right\} \end{aligned} \tag{51}$$

are equivalent to each other and to the more conventional expression of Eq. (24). One advantage of the $XY$-form, Eq. (51), $V_{XY}(\vec{r}_1,\vec{r}_2)$, is that the unlike boson scattering length $a_u$ only occurs in the spin-spin term. As a consequence a mixed spin channel Feshbach resonance will vary only the $XY$spin-spin coupling. In general, a Feshbach resonance occurs when the incident particle channel becomes degenerate with the quasi-bound state of another collision channel. Hence a particular resonance will either vary $a_\uparrow$, or $a_\downarrow$ or $a_u$. A mixed spin channel resonance of magnetic field width $\Delta B$ around magnetic field strength $B_{res}$ varies the unlike scattering length $a_u$ as

$$a_{u,res}(B) = a_u\left[1 - \frac{\Delta B}{B - B_{res}}\right]\,, \tag{52}$$

where $a_u$ is the background scattering length that varies slowly with magnetic field (on the magnetic field scale of $B_{hf}$. The Feshbach variation thereby adds an effective interaction potential

$$\Delta V_{XY}\left(\vec{r}_1,\vec{r}_2\right)=\left(\frac{\Delta B}{B_{res}-B}\right)\left(\frac{4\pi\hbar^2 a_u}{m}\right)\delta\left(\vec{x}_1-\vec{x}_2\right)\left(s_{1,x}s_{2,x}+s_{1,y}s_{2,y}\right) \quad (53)$$

to the above $XY$ form of the spin-dependent particle-particle interaction Eq. (51).

In terms of the magnetic form of the inter-particle interactions,

$$V_{I(X,Y)}=V_{o,I(X,Y)}\left(\vec{x}_1-\vec{x}_2\right)+V_{s,I(X,Y)}\left(\vec{r}_1,\vec{r}_2\right), \quad (54)$$

where $V_{o,I(XY)}=[4\pi\hbar^2/m]\delta\left(\vec{x}_1-\vec{x}_2\right)a_{o,I(X,Y)}$ in which

$$\begin{aligned} a_{o,I} &= \frac{a_\uparrow+a_\downarrow+2a_u}{4}, \\ a_{o,XY} &= \frac{a_\uparrow+a_\downarrow}{2}, \end{aligned} \quad (55)$$

denote the Ising and XY expressions of the spin independent scattering length. The spin interactions take the usual form $V_{s,I(XY)}\left(\vec{r}_1,\vec{r}_2\right)=\mathbf{s}_1\cdot\mathbf{h}_{2,I(XY)}\left(\vec{x}_1\right)+\mathbf{s}_2\cdot\mathbf{h}_{1,I(XY)}\left(\vec{x}_2\right)$ with $\mathbf{h}_{i,I(XY)}\left(\vec{x}\right)=\delta\left(\vec{x}-\vec{x}_i\right)\mathbf{m}_{i,I(XY)}$ and

$$\begin{aligned} \mathbf{m}_{i,I} &= m_o\mathbf{z}+\left(m_\parallel-m_\perp\right)\mathbf{z}\ \left(\mathbf{s}_i\cdot\mathbf{z}\right), \\ \mathbf{m}_{i,XY} &= m_o\mathbf{z}+\left(m_\perp-m_\parallel\right)\mathbf{z}\times\left(\mathbf{s}_i\times\mathbf{z}\right), \end{aligned} \quad (56)$$

with moment parameters $(m_o,m_\parallel,m_\perp)$ defined in Eq. (38).

### *3.4. Spin dependence of alkali atom interactions and the degenerate internal state approximation*

The spin-dependence of the alkali-atom interactions stems from the exchange of valence electrons. As two alkali-nuclei approach each other to nanometer and sub-nanometer distance, their valence electrons, now encircling the two closely-spaced nuclei, become strongly correlated. If these electrons are indistinguishable, i.e., if their spins align in a triplet sate, the likelihood of finding them simultaneously in each others vicinity is reduced by virtue of the Pauli principle. Pauli exclusion then reduces the Coulomb energy shift in the inter-atomic potential. In contrast, spin singlet electrons can approach each other more closely, shifting the inter-atomic potential upward. Hence, the triplet potential $V_T$ is generally deeper than the singlet potential $V_S$. The overall interaction of atoms can be expressed by an inter-atomic potential operator

$$V\left(\mathbf{r}_1,\mathbf{r}_2\right)=V_T\left(\left|\mathbf{x}_1-\mathbf{x}_2\right|\right)\hat{\Pi}_{e,T}+V_S\left(\left|\mathbf{x}_1-\mathbf{x}_2\right|\right)\hat{\Pi}_{e,S}, \quad (57)$$

where the $\mathbf{r}$ represent both the spatial coordinates $\mathbf{x}$, and spin, and $\hat{\Pi}_{e,T}$ , $\hat{\Pi}_{e,S}$ denote the projection operators for the electron triplet $S=1$ and singlet $S=0$ states. When acting upon a triplet state, the square of the total electron spin operator, $\mathbf{S}_e^2=\frac{3}{2}+2\mathbf{s}_{e,1}\cdot\mathbf{s}_{e,2}$ yields an eigenvalue of 2 (i.e. $S\left(S+1\right)$ with $S=1$). Acting upon a singlet state, the same operator gives zero, so that the triplet projection operator takes the form

$$\hat{\Pi}_{e,T}=\frac{\mathbf{S}_e^2}{2}=\frac{3}{4}+\mathbf{s}_{e,1}\cdot\mathbf{s}_{e,2}. \quad (58)$$

Since $\hat{\Pi}_{e,T} + \hat{\Pi}_{e,S} = 1$, the singlet projection operator is equal to

$$\hat{\Pi}_{e,S} = 1 - \hat{\Pi}_{e,T} = \frac{1}{4} - \mathbf{s}_{e,1} \cdot \mathbf{s}_{e,2} \ . \tag{59}$$

With Eqs. (58) and (59), the interatomic interaction potential operator Eq. (57) reads

$$\begin{aligned} V(\mathbf{r}_1, \mathbf{r}_2) = & \frac{1}{4}\left[3V_T(|\mathbf{x}_1 - \mathbf{x}_2|) + V_S(|\mathbf{x}_1 - \mathbf{x}_2|)\right] \\ & + \left[V_T(|\mathbf{x}_1 - \mathbf{x}_2|) - V_S(|\mathbf{x}_1 - \mathbf{x}_2|)\right] \mathbf{s}_{e,1} \cdot \mathbf{s}_{e,2} \ . \end{aligned} \tag{60}$$

The depth of the $V_S$ and $V_T$ potentials ($\sim$ electron Volt - $10^4 K$) greatly exceeds the energy of the Zeeman spin interactions $\sim a_{hf}$, tens of $mK$). Inside the potential well, $r < r_1$, the hyperfine interaction can be neglected whereas in the outer region, $r > r_1$, the hyperfine interaction determines the spin state of the collision channel. The exchange interaction, $(V_T - V_S)\, \vec{s}_{e,1} \cdot \vec{s}_{e,2}$ also falls off rapidly (exponentially) in the outer region. One can then calculate the scattering wavefunction while omitting the Zeeman terms in $r < r_1$ and treating the exchange interaction in the region $r > r_1$ as a perturbation term. In lowest order perturbation the T-matrix should then have a contribution proportional to $\vec{s}_{e,1} \cdot \vec{s}_{e,2}$ evaluated for the initial and outgoing channels. The spin-independent and the $\vec{s}_{e,1} \cdot \vec{s}_{e,2}$-parts of the T-matrix should reproduce the correct triplet and singlet scattering lengths $a_S$ and $a_T$ in the limit of vanishing magnetic field and hyperfine energy. In this approximation, the low energy $i, j \to k, l$ transition matrix element then takes the form,

$$T_{i,j;k,l} \approx \left(\frac{4\pi\hbar^2}{m}\right) \langle i, j | \overline{a} + a_- \vec{s}_{e,1} \cdot \vec{s}_{e,2} | k, s \rangle \ , \tag{61}$$

where $\overline{a}$ denotes the scattering length averaged over the singlet and triplet states,

$$\overline{a} = \left(\frac{3a_T + a_S}{4}\right) \ , \tag{62}$$

and where $a_-$ represents the difference scattering length,

$$a_- = a_T - a_S \quad . \tag{63}$$

This approximation is called the Degenerate Internal State (DIS) approximation. While it was primarily designed for calculating the two-body loss rate of atoms occupying specific hyperfine states in an external magnetic field. In that case, if the magnetic field is comparable to the hyperfine field, the above formula does not work very well as the wavefunction of the outgoing channel is not very well approximated by the zero energy wave function. We are not considering lossy channels, which will not be there if the hyperfine states are chosen carefully as described in the previous section. We are only considering the cases $i = k, j = l$ or $i = l, j = k$ with $i, j = \uparrow, \downarrow$, for which the incident and final channel wavefunctions have the same low energy value. Even in that case, the approximation is not always satisfied, particularly for atoms that have a naturally large scattering length at zero magnetic field, such as $^7Li$ [35] and $^{123}$Cs [36] and for higher magnetic field values. We expect that the treatment, may, however, yield a reasonable approximation for magnetic field values near such low magnetic field resonances as the $9G$ resonance observed in $^{87}Rb$ [37].

In the DIS approximation, we can calculate the above defined scattering lengths explicitly

$$\begin{aligned} a_\uparrow &= \bar{a} + a_- \left\langle \uparrow\uparrow \left| \mathbf{s}_{e,1} \cdot \mathbf{s}_{e,2} \right| \uparrow\uparrow \right\rangle, \\ a_\downarrow &= \bar{a} + a_- \left\langle \downarrow\downarrow \left| \mathbf{s}_{e,1} \cdot \mathbf{s}_{e,2} \right| \downarrow\downarrow \right\rangle, \\ a_D &= a_- \left\langle \uparrow\downarrow \left| \mathbf{s}_{e,1} \cdot \mathbf{s}_{e,2} \right| \uparrow\downarrow \right\rangle, \\ a_x &= a_- \left\langle \uparrow\downarrow \left| \mathbf{s}_{e,1} \cdot \mathbf{s}_{e,2} \right| \downarrow\uparrow \right\rangle. \end{aligned} \tag{64}$$

in terms of the single electron spin matrix elements $\mathbf{s}_{e,\uparrow} = \langle \uparrow | \mathbf{s}_e | \uparrow \rangle$, $\mathbf{s}_{e,\downarrow} = \langle \downarrow | \mathbf{s}_e | \downarrow \rangle$,

$$\left\langle \uparrow\uparrow \left| \mathbf{s}_{e,1} \cdot \mathbf{s}_{e,2} \right| \uparrow\uparrow \right\rangle = \mathbf{s}_{e,\uparrow} \cdot \mathbf{s}_{e,\uparrow}, \tag{65}$$

$$\left\langle \downarrow\downarrow \left| \mathbf{s}_{e,1} \cdot \mathbf{s}_{e,2} \right| \downarrow\downarrow \right\rangle = \mathbf{s}_{e,\downarrow} \cdot \mathbf{s}_{e,\downarrow}, \tag{66}$$

$$\left\langle \uparrow\downarrow \left| \mathbf{s}_{e,1} \cdot \mathbf{s}_{e,2} \right| \uparrow\downarrow \right\rangle = \mathbf{s}_{e,\uparrow} \cdot \mathbf{s}_{e,\downarrow}. \tag{67}$$

The exchange spin matrix element involves spin-flip matrix elements of the type $\langle \uparrow | \mathbf{s}_e | \downarrow \rangle = \mathbf{s}_{e,\uparrow\downarrow}$, so that

$$\left\langle \uparrow\downarrow \left| \mathbf{s}_{e,1} \cdot \mathbf{s}_{e,2} \right| \downarrow\uparrow \right\rangle = \mathbf{s}_{e,\uparrow\downarrow} \cdot \mathbf{s}_{e,\downarrow\uparrow}\,. \tag{68}$$

The spin-spin interaction parameters,

$$\begin{aligned} a_{o,I} &= \overline{a} + \frac{a_-}{4} \left( \mathbf{s}_{e,\uparrow} + \mathbf{s}_{e,\downarrow} \right) \cdot \left( \mathbf{s}_{e,\uparrow} + \mathbf{s}_{e,\downarrow} \right), \\ m_{s,o} &= \frac{2\pi\hbar^2}{m} a_- \left( \mathbf{s}_{e,\uparrow} + \mathbf{s}_{e,\downarrow} \right) \cdot \left( \mathbf{s}_{e,\uparrow} - \mathbf{s}_{e,\downarrow} \right), \\ m_{s,\parallel} &= \frac{2\pi\hbar^2}{m} a_- \left( \mathbf{s}_{e,\uparrow} - \mathbf{s}_{e,\downarrow} \right) \cdot \left( \mathbf{s}_{e,\uparrow} - \mathbf{s}_{e,\downarrow} \right), \\ m_{s,\perp} &= \frac{2\pi\hbar^2}{m} a_- 2\mathbf{s}_{e,\uparrow\downarrow} \cdot \mathbf{s}_{e,\downarrow\uparrow}, \end{aligned} \tag{69}$$

then depend on the single electron spin-flip and spin matrix elements.

As the electron spin expectation values depend on the external magnetic field, the interaction parameters do as well. To express the dependence explicitly, we cast the expressions in parametric form, choosing the electron spin inclination angles $\theta_\uparrow$, $\theta_\downarrow$ of the 'up' and 'down' hyperfine states of Eq. (19) as variable. For notational convenience we introduce external magnetic field-dependent spin factors $\mathcal{S}_{m,n}(b)$ with $m$ and $n$ equal to $+1$ or $-1$,

$$\begin{aligned} \mathcal{S}_{m,n}(b) &= \left( \mathbf{s}_{e,\uparrow} + m\vec{s}_{e,\downarrow} \right) \cdot \left( \mathbf{s}_{e,\uparrow} + n\mathbf{s}_{e,\downarrow} \right), \\ &= \left[ \frac{\cos(\theta_\uparrow) + m\cos(\theta_\downarrow)}{2} \right] \left[ \frac{\cos(\theta_\uparrow) + n\cos(\theta_\downarrow)}{2} \right]. \end{aligned} \tag{70}$$

In addition, we introduce the exchange spin factor, $\mathcal{S}_x(b)$, with $\mathcal{S}_x(b) = 2\mathbf{s}_{e,\uparrow\downarrow} \cdot \mathbf{s}_{e,\downarrow\uparrow}$. To determine its value we make assumptions about how the $|\uparrow\rangle$ and $|\downarrow\rangle$ are chosen: We assume that their respective $m_f$-values differ by one unit (if not, $\mathbf{s}_{e,\uparrow\downarrow} = \mathbf{s}_{e,\downarrow\uparrow} = 0$) and we choose the $|\uparrow\rangle$ to have the highest $m_f$. We also assume that both states are chosen among the states with Zeeman energy-curves that slope down at high magnetic fields

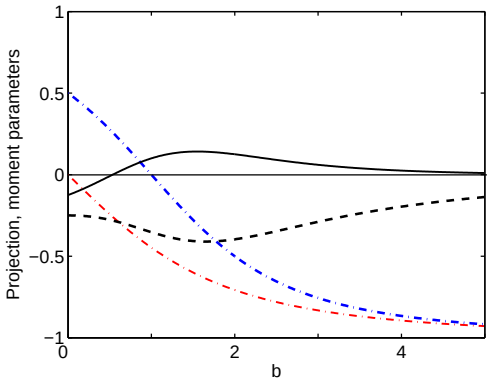


**Figure 3.** The graph shows the magnetic field dependence ($b = B/B_{hf}$) of the moment parameters as calculated in the DIS approximation for $i = 3/2$, $|\uparrow\rangle = |f = 1, m_f = 0\rangle$ and $|f = 1, m_f = -1\rangle$. The full line shows $m_0/\left(\pi\hbar^2/m\right) a_-$, whereas the dashed line shows $2\left(m_\parallel - m_\perp\right)/\left(\pi\hbar^2/m\right) a_-$, where $a_-$ represents the difference of the zero magnetic field triplet ($a_T$) and singlet ($a_S$) scattering lengths, $a_- = a_T - a_S$. The dashed lines show the cosine of the electron spin projection angle of the 'up' and 'down' hyperfine states. The higher lying dashed line plots $\cos(\theta_\downarrow)$, the lower dashed line plots $\cos(\theta_\uparrow)$. It is near the $b = 1$ at which the down state electron spin changes its direction from parallel to antiparellel to the external magnetic field that $m_o$ changes sign and $|m_\parallel - m_\perp|$ is maximized.

(either the $f^-$-states or the stretched electron spin-down state, $|f = f^+, m_f = -f^+\rangle$). In that case the $|\uparrow\rangle$-state has the lower Zeeman energy. With this convention, we find

$$\mathcal{S}_x(b) = \left[\frac{1+\cos(\theta_\uparrow)}{2}\right]\left[\frac{1-\cos(\theta_\downarrow)}{2}\right], \tag{71}$$

where the projection of the inclination angle varies with the external magnetic field as in Eq. (19). In terms of the $\mathcal{S}$–spin factors, the effective pseudospin interaction parameters take on simple forms

$$\begin{aligned} a_{o,I} &= \bar{a} + \frac{a_-}{4}\,\mathcal{S}_{+,+}(b)\ , \\ m_{s,o} &= \frac{2\pi\hbar^2}{m} a_-\,\mathcal{S}_{+,-}(b)\ , \\ m_{s,\parallel} &= \frac{2\pi\hbar^2}{m} a_-\,\mathcal{S}_{-,-}(b)\ , \\ m_{s,\perp} &= \frac{2\pi\hbar^2}{m} a_-\,\mathcal{S}_x(b)\ . \end{aligned} \tag{72}$$

Note that all three moment parameters are proportional to the difference scattering length $a_-$.

Figure 3 plots the magnetic field dependence ($b = B/B_{hf}$ as defined above Eq. (10)) of the relevant moment-parameters as calculated in the DIS approximation for the special case, $i = 3/2$, $|\uparrow\rangle = |f = 1, m_{ff} = 0\rangle$ and $|f = 1, m_f = -1\rangle$ (i.e., the second and third lowest Zeeman energy levels of Fig. 1). The full line plots $m_o$, whereas the

dash-dotted line plots $2(m_{\parallel}-m_{\perp})$, both in units of $(\pi\hbar^2 a_-/m)$. For reference, note that the Ising form of the spin $\frac{1}{2}$ boson particle-particle interaction takes the form

$$V(\vec{r}_1,\vec{r}_2)=\delta(\vec{x}_1-\vec{x}_2)\left[\lambda_0+m_o s_{1,z}s_{2,z}+2\left(m_{\parallel}-m_{\perp}\right)s_{1,z}s_{2,z}\right], \tag{73}$$

where $\lambda_0$ denotes the spin-independent interaction strength in the Ising form, $\lambda_0 = (\pi\hbar^2/m)\left[a_\uparrow + a_\downarrow + 2a_u\right]$. Note that $m_o$ changes sign near $b = 0.535$, so that there exists an external magnetic field strength at which the spin-independent effective short-range magnetic field carried by the interacting particles can be made to vanish (without having to take recourse to a Feshbach resonance). The Ising spin-spin interaction coefficient does not change sign but it's magnitude is maximized at a magnetic field $b \sim 1.75$. The precise values of the magnetic fields at which the interaction parameters exhibit this behavior may be different, but we expect the DIS-approximation to give the correct qualitative behavior even if the DIS-approximation is not expected to be accurate at higher magnetic field values.

## 4. A controllable $N$ boson quantum magnet

The spin-spin forms of the effective inter-particle interactions reveal the analogy with magnetic systems. As an illustration we consider a specific system that promises a particularly powerful and interesting simulation of a quantum magnet: N indistinguishable bosons occupying two hyperfine spin states $|\uparrow\rangle$, $|\downarrow\rangle$, confined by a tight spatial potential (which could be a single well of an optical lattice). We assume that both $|\uparrow\rangle$ and $|\downarrow\rangle$ experience the same trapping potential $V_\uparrow(\vec{x}) = V_\downarrow(\vec{x}) = V_T(\vec{x})$ of single-particle ground state $\chi_T(\vec{x})$ and single particle ground state energy $e_T$. When $e_T$ exceeds all other energy-per-particle values and the system relaxed to its motional ground state, all of the $N$ bosons occupy the $\chi_T$-orbital and the spatial degrees of freedom are 'frozen', allowing only spin dynamics. We also assume that the $|\uparrow\rangle$ and $|\downarrow\rangle$ experience a coherent two-photon Raman coupling which can be effected by pulses of near-resonant lasers (or by means of an oscillating magnetic field). The resonant Raman coupling also introduces a detuning $\epsilon$ which acts as an effective energy difference between $|\uparrow\rangle$ and $|\downarrow\rangle$ and the Raman coupling is described by a term

$$\begin{aligned}&\sum_{j=1}^{N}\left[-E_R(t)\left(|\downarrow\rangle_j\ {}_j\langle\uparrow|+|\uparrow\rangle_j\ {}_j\langle\downarrow|\right)+\frac{\epsilon}{2}\left(|\uparrow\rangle_j\ {}_j\langle\uparrow|-|\downarrow\rangle_j\ {}_j\langle\downarrow|\right)\right]\\&=-2E_R(t)\sum_{j=1}^{N}s_{j,x}+\epsilon\sum_{j=1}^{N}s_{j,z},\end{aligned} \tag{74}$$

in the Hamiltonian. In the above expression, $E_R$ denotes the Rabi-coupling energy which varies in time if the coupling is caused by a pulse.

The premise of a trapping potential sufficiently tight to freeze out the spatial degrees of freedom translates into an $N$-particle wavefunction of the type

$$\Psi(\vec{r}_1,\vec{r}_2,....,\vec{r}_N)=\chi_T(\vec{x}_1)\chi_T(\vec{x}_2)...\chi_T(\vec{x}_N)\ \left|S^N(\vec{s}_1,\vec{s}_2,...\vec{s}_N)\right\rangle, \tag{75}$$

where $\left|S^N\right\rangle$ denotes the spin state of the $N$-boson system. By virtue of permutation symmetry – the full wavefunction has to be even under permutation of the full $\vec{r}=(\vec{x},\vec{s})$ coordinates of any pair of particles – the $\left|S^N\right\rangle$ spin state is required to be even with respect to the permutation of any pair of spin variables $i$ and $j$. This condition limits the spin states to the manifold of maximal spin magnitude. Specifically, if we introduce the total spin operator, $\mathbf{S}^N=\sum_{j=1}^N \mathbf{s}_j$, then $\mathbf{S}^N\cdot\mathbf{S}^N\left|S^N\right\rangle=\frac{N}{2}\left(\frac{N}{2}+1\right)\left|S^N\right\rangle$, corresponding to a total spin magnitude $\frac{N}{2}$, i.e., all pseudo-spins aligned. Hence, the spin state is a linear combination of $S^N=\frac{N}{2}$ states of total spin projection $M_S=-\frac{N}{2},...,\frac{N}{2}$, $\left|S^N=\frac{N}{2},M_S\right\rangle$ with $S_z^N\left|S^N=\frac{N}{2},M_S\right\rangle=M_S\left|S^N=\frac{N}{2},M_S\right\rangle$. The $M_S=\frac{N}{2}$ is an $N$-spin stretched state.

$$\left|S^N=\frac{N}{2},M_S=\frac{N}{2}\right\rangle=\left|\uparrow\right\rangle_1\ \left|\uparrow\right\rangle_2\ ...\ \left|\uparrow\right\rangle_N, \tag{76}$$

In deriving the expression for the total energy $E$ of the $N$ interacting boson system, we use the Ising spin-spin form of the short-range particle-particle interaction. Integrating out the position variables explicitly, we encounter a volume $v$, the 'trap volume' that characterizes the 'tightness' of the confining $V_T$,

$$\frac{1}{v}=\int d^3\vec{x}\left|\chi_T\left(\vec{x}\right)\right|^4, \tag{77}$$

For instance, the spin-independent interaction energy per particle, $e_0$, is inversely proportional to the trap volume $v$ and proportional to the spin-independent interaction strength in the Ising form, $\lambda_0=(4\pi\hbar^2/m)\left[\frac{a_\uparrow+a_\downarrow+2a_u}{4}\right]$,

$$e_0=\frac{\lambda_0}{v}. \tag{78}$$

The analogous spin-interaction energies per particle are given by the expressions

$$\begin{aligned}\epsilon_o&=\frac{m_o}{v}=\frac{4\pi\hbar^2}{m}\left(\frac{a_\uparrow-a_\downarrow}{2}\right)\frac{1}{v},\\ \epsilon_I&=\frac{2\left(m_\parallel-m_\perp\right)}{v}=\frac{4\pi\hbar^2}{m}\left(a_\uparrow+a_\downarrow-2a_u\right)\frac{1}{v}.\end{aligned} \tag{79}$$

The total many-body energy, $E$, takes the form

$$\begin{aligned}E=N\left[e_T+\frac{(N-1)}{2}e_0\right]&+(N-1)\,\epsilon_o\sum_{j=1}^N\left\langle S^N\left|s_{j,z}\right|S^N\right\rangle\\ &+\frac{\epsilon_I}{2}\sum_{i\neq j}\left\langle S^N\left|s_{j,z}s_{j,z}\right|S^N\right\rangle+\sum_{j=1}^N\left\langle S^N\left|(-2\epsilon_R s_{j,x}+\epsilon s_{j,z})\right|S^N\right\rangle,\end{aligned} \tag{80}$$

so that the integration over the position variable with short-range interactions maps the $N$ spin-1/2 boson problem into that of $N$ 1/2 spins coupled via an infinite range spin-spin interaction. By adding and subtracting

$$\frac{\epsilon_I}{2}\sum_{j=1}^N s_{j,z}s_{j,z}=\frac{N\epsilon_I}{8}, \tag{81}$$

we cast the Hamiltonian in terms of the total spin-operator $\mathbf{S}^N = \sum_{j=1}^{N} \mathbf{s}_j$. We also define effective magnetic fields that are $c$ numbers,

$$\begin{aligned} \mathbf{H}_o &= (N-1)\,\mathbf{z}\epsilon_o \\ \mathbf{H}_R &= -2\epsilon_R \mathbf{x} + \epsilon \mathbf{z} \end{aligned} \tag{82}$$

The energy $E$, up to an unimportant shift, $E' = E - N\left[e_T + (N-1)\,\frac{e_0}{2}\right] - \frac{N\epsilon_I}{8}$, then takes the form

$$E' = \left\langle S^N \left| \mathbf{S}^N \cdot (\mathbf{H}_o + \mathbf{H}_R) + \frac{\epsilon}{2} S_z^N S_z^N \right| S^N \right\rangle, \tag{83}$$

reminiscent of the Hamiltonian of magnetic single domain grains with anisotropic spin-spin interactions [38]. Chudnovsky and Gunther had pointed out that the anisotropy can set conditions under which we expect macroscopic quantum tunneling: sufficiently strong exchange interactions force the individual spins to align into a macroscopic spin vector, the anisotropy can give local energy minima corresponding to two distinct directions of the macroscopic spin and quantum mechanically, the macroscopic spin can travel through a classically forbidden region giving tunneling although the expected rate for such processes are exponentially suppressed with the number of spins. In the $N$-boson quantum magnet, the alignment is enforced by permutation symmetry, the anisotropy caused by the Ising (or XY) nature of the effective inter-particle interactions and the number of bosons can, in principle, be controlled experimentally.

We recognize the operator in the spin bracket of Eq. (83) as the spin Hamiltonian $\hat{H}$. The Heisenberg equation of motion for the total spin operator,

$$i\hbar \frac{d\mathbf{S}^N}{dt} = \left[\mathbf{S}^N, \hat{H}\right]_- = i\mathbf{S}^N \times [\mathbf{H}_o + \mathbf{H}_R] + i\epsilon_I \mathbf{S}_{\|}^N \left(\mathbf{S}^N \cdot \mathbf{z}\right) \ , \tag{84}$$

where $\mathbf{S}_{\|}^N$ denotes the part of the total spin vector that points in the direction of the magnetic field, $\mathbf{S}_{\|}^N = \mathbf{z}\ \left(\mathbf{S}^N \cdot \mathbf{z}\right)$, yields an Ehrenfest type of equation for the total spin expectation value if we take its expectation value. We can write the resulting equation as a Landau-Lifshitz equation (without damping term) [39],

$$\frac{d}{dt}\langle \mathbf{S^N} \rangle = \frac{1}{\hbar} \langle \mathbf{S}^N \times \mathbf{H}_{total} \rangle \ , \tag{85}$$

where the total magnetic field $\mathbf{H}_{total}$ includes the Raman coupling effective field, the the effective, spin-independent short-range field carried by the other particles and the contribution caused by the Ising spin-spin interactions,

$$\mathbf{H}_{total} = \mathbf{H}_o + \mathbf{H}_R + \epsilon_I \mathbf{S}_{\|}^N \left(\mathbf{S}_N \cdot \mathbf{z}\right) \ . \tag{86}$$

In the absence of Raman coupling $\mathbf{H}_R = 0$ the total magnetic field $\mathbf{H}_{total}$ points in the z-direction and all the spin expectation vector can do is precess around the z-direction. In fact, the derivative of the expectation value of any power of $S_z^N$ vanishes so that the conservation of up and down particles ensures that the distribution of the spin up and spin down particles will remain constant in time precluding collective tunneling of the spin in the absence of Raman coupling. A Raman pulse can then precisely control and initiate the macroscopic quantum tunneling while leaving the

other assumptions and parameters of the system untouched. In addition to tunneling, the ground state of the system can be a superposition of two distinct states in each of which the total spin points in different directions. That Raman-coupled (or Josephson-coupled) two-component BEC systems can take on macroscopic Schrodinger cat states was pointed out in [40] and worked out in [41] – we simply determine the interaction parameters and indicate how these can be controlled. The Raman control provides an important advantage to the N-boson quantum magnet over the double-well proposals for realizing macroscopic quantum tunneling and creating macrocopic Schrodinger cat states. Varying the potential barrier in a double well system to control the tunneling can also render the two-state approximation invalid and lead to unwanted excitations.

Observing the coherent oscillations of the total spin that is quantum tunneling can also test fundamental aspects of quantum mechanics (against macroscopic realism) by verifying Legget-Garg inequalities [42]. In addition, the $N$-boson quantum magnet spin dynamics can also explore spin squeezing, non-classical quantum evolution near unstable trajectories [43] and, when the Ising interaction is eliminated by a Feshbach resonance, realize the Burnett-Holand proposal for Heisenberg limited interferometry [44] by using the Raman pulse as a beam-splitter. These connections become obvious using the spin-spin form of the inter-particle interactions which also reveal the control that routine cold atom knobs such as the intensity of the confining potential, the detuning of the Raman coupling pulse and the magnetic field of a Feshbach resonance can exercise.

## 5. Conclusions

In conclusion, we described the effective spin-dependent interactions of ultra-cold alkali atoms occupying two distinct hyperfine states in an external magnetic field. The magnetic field lifts the degeneracy of the atomic Zeeman levels and permits the selection of two hyperfine states to act as the effective 'spin-up' and 'spin-down' states of the particles so the atoms can mimic the behavior of magnetic spin-$\frac{1}{2}$ particles. We described the spin-dependent effective interaction as a spin-spin interaction. The form of the effective spin-spin interaction depends explicitly on the quantum statistics of the interacting particles. As a consequence of the zero-range nature of the interaction, the interaction of spin-$\frac{1}{2}$ bosons can be described as an Ising or, alternatively, as an $XY$-coupling. The parameters of the spin-spin interaction depend on the scattering lengths of the relevant binary alkali atom collision channels in the external magnetic field. For relatively low values of the magnetic field (sufficiently large to cause a Zeeman level splitting that permits the selection of two hyperfine levels) we calculated the parameters as a function of the external magnetic field in the Degenerate Internal State (DIS) approximation. We illustrated the advantage of the spin-spin interaction form by mapping the system of N spin-$\frac{1}{2}$ bosons in a tight trapping potential on that of N spin-$\frac{1}{2}$ spins coupled via an infinite range interaction. The explicit expressions reveal which parameters of the spin Hamiltonian can be controlled and how. The spin Hamiltonian also suggests that the N-boson quantum magnet provides an intriguing

laboratory for the exploration of fundamental quantum studies. The list of promising uses include the study of collective quantum spin tunneling (which can be used for testing fundamental aspects of quantum mechanics), the controlled observation and utilization of spin squeezing and the creation and study of highly non-classical states.

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